# Calculation of the spin-dependent wavefunction in a magnetic sample, in the reflection geometry

Brian B. Maranville*
*NIST Center for Neutron Research*
*100 Bureau Drive, Gaithersburg MD USA 20899*
(Dated: August 5, 2013)

The theory of polarized neutron reflectometry has long been worked out, and the amplitude of the reflected and transmitted waves (at large distances from the sample) can be easily calculated using available computer code. When using the one-dimensional reflectivity theory in the special case of the distorted-wave Born approximation (DWBA), the amplitudes of the wavefunctions are needed inside the sample as well, and in this paper we describe the implementation of this calculation.

## SPIN-POLARIZED NEUTRON REFLECTIVITY

The theory of polarized neutron reflectivity is thoroughly described in the literature [1]. The two coupled equations describing the spin-dependent wavefunction are

$$\begin{aligned}\left[\frac{\partial^2}{\partial z^2} + \frac{Q^2}{4} - 4\pi\rho_{++}(z)\right]\psi_+(z) - 4\pi\rho_{+-}(z)\psi_-(z) = 0\\ \left[\frac{\partial^2}{\partial z^2} + \frac{Q^2}{4} - 4\pi\rho_{--}(z)\right]\psi_-(z) - 4\pi\rho_{-+}(z)\psi_+(z) = 0\end{aligned} \tag{1}$$

where

$$\begin{pmatrix}\rho_{++} & \rho_{+-}\\ \rho_{-+} & \rho_{--}\end{pmatrix} = \begin{pmatrix}Nb + Np_z & Np_x - iNp_y\\ Np_x + iNp_y & Nb - Np_z\end{pmatrix} \tag{2}$$

The $\hat{z}$ direction in the sample coordinate system is the surface normal, which is of course also the direction of the momentum transfer $\vec{Q}$. As described in [1], the two coupled equations can be combined to give two fourth-order uncoupled equations, and if we use a solution of the form $\psi = \exp(Sz)$ the four roots of $S$ are

$$\begin{aligned}S_1 &= \sqrt{4\pi(Nb + Np) - Q^2/4}\\ S_2 &= -S_1\\ S_3 &= \sqrt{4\pi(Nb - Np) - Q^2/4}\\ S_4 &= -S_3\end{aligned} \tag{3}$$

and the total wavefunction is the combination of one that is spin-up and one that is spin-down (in the sample reference frame.)

$$\begin{aligned}\Psi(z) &= \begin{pmatrix}\psi_+(z)\\ \psi_-(z)\end{pmatrix}\\ \psi_+(z) &= \sum_{j=1}^{4} C_j e^{S_j z}\\ \psi_-(z) &= \sum_{j=1}^{4} D_j e^{S_j z}\end{aligned} \tag{4}$$

The coupling from the first equation leads to a relationship between the coefficients of the two sub-wavefunctions:

$$D_j = \mu_j C_j \tag{5}$$

where

$$\begin{aligned}\mu_1 &= \tfrac{1+\cos\theta_M + i\sin\theta_M\cos\phi_M - \sin\theta_M\sin\phi_M}{1+\cos\theta_M - i\sin\theta_M\cos\phi_M + \sin\theta_M\sin\phi_M}\\ \mu_2 &= \mu_1\\ \mu_3 &= \tfrac{-1+\cos\theta_M + i\sin\theta_M\cos\phi_M - \sin\theta_M\sin\phi_M}{-1+\cos\theta_M - i\sin\theta_M\cos\phi_M + \sin\theta_M\sin\phi_M}\\ \mu_4 &= \mu_3\end{aligned} \tag{6}$$

($\theta_M$ is the in-plane $\hat{x}$-$\hat{y}$ rotation vector, zero at $\hat{x}$, $\phi_M$ is the out-of-plane component along $\hat{z}$), but in the case where the $z$-component of the magnetization is held to be zero (or constant through fronting/sample/backing) the angle $\phi_M$ is zero, and $\mu$ is

$$\begin{aligned}\mu_1 &= \mu_2 = e^{i\theta_M}\\ \mu_3 &= \mu_4 = -e^{i\theta_M}\end{aligned} \tag{7}$$

Then we can write a column vector for $\Psi(z)$ and $\Psi'(z)$ representing all the wavefunction terms that are continuous in the solution, as the second-order Schrödinger equation requires.

$$\begin{pmatrix}\psi_+(z)\\ \psi_-(z)\\ \psi'_+(z)\\ \psi'_-(z)\end{pmatrix} = \chi\begin{pmatrix}C_1\\ C_2\\ C_3\\ C_4\end{pmatrix} \tag{8}$$

where

$$\chi = \begin{pmatrix}e^{S_1 z} & e^{-S_1 z} & e^{S_3 z} & e^{-S_3 z}\\ \mu e^{S_1 z} & \mu e^{-S_1 z} & -\mu e^{S_3 z} & -\mu e^{-S_3 z}\\ S_1 e^{S_1 z} & -S_1 e^{-S_1 z} & S_3 e^{S_3 z} & -S_3 e^{-S_3 z}\\ \mu S_1 e^{S_1 z} & -\mu S_1 e^{-S_1 z} & -\mu S_3 e^{S_3 z} & \mu S_3 e^{-S_3 z}\end{pmatrix} \tag{9}$$

or, separating out the z-dependent terms within a layer

$$\chi = \begin{pmatrix}1 & 1 & 1 & 1\\ \mu & \mu & -\mu & -\mu\\ S_1 & -S_1 & S_3 & -S_3\\ \mu S_1 & -\mu S_1 & -\mu S_3 & \mu S_3\end{pmatrix}_l \begin{pmatrix}e^{S_1 z} & 0 & 0 & 0\\ 0 & e^{-S_1 z} & 0 & 0\\ 0 & 0 & e^{S_3 z} & 0\\ 0 & 0 & 0 & e^{-S_3 z}\end{pmatrix} \tag{10}$$

The inverse of the first ($z$-independent) matrix above allows one to calculate the $C_j$ in terms of $\Psi(z = 0)$

$$\frac{1}{4}\begin{pmatrix}1 & \frac{1}{\mu} & \frac{1}{S_1} & \frac{1}{\mu S_1}\\ 1 & \frac{1}{\mu} & \frac{-1}{S_1} & \frac{-1}{\mu S_1}\\ 1 & \frac{-1}{\mu} & \frac{1}{S_3} & \frac{-1}{\mu S_3}\\ 1 & \frac{-1}{\mu} & \frac{-1}{S_3} & \frac{1}{\mu S_3}\end{pmatrix}\begin{pmatrix}\psi_+(0)\\ \psi_-(0)\\ \psi'_+(0)\\ \psi'_-(0)\end{pmatrix} = \begin{pmatrix}C_1\\ C_2\\ C_3\\ C_4\end{pmatrix} \tag{11}$$

Note that substituting the left side of Eq. 11 into the right side of Eq. 8 gives the transfer matrix:

$$\begin{pmatrix}\psi_+(z)\\ \psi_-(z)\\ \psi'_+(z)\\ \psi'_-(z)\end{pmatrix} = A\begin{pmatrix}\psi_+(0)\\ \psi_-(0)\\ \psi'_+(0)\\ \psi'_-(0)\end{pmatrix} \tag{12}$$

$$A = \frac{1}{4}\begin{pmatrix} e^{S_1 z} & e^{-S_1 z} & e^{S_3 z} & e^{-S_3 z}\\ \mu e^{S_1 z} & \mu e^{-S_1 z} & -\mu e^{S_3 z} & -\mu e^{-S_3 z}\\ S_1 e^{S_1 z} & -S_1 e^{-S_1 z} & S_3 e^{S_3 z} & -S_3 e^{-S_3 z}\\ \mu S_1 e^{S_1 z} & -\mu S_1 e^{-S_1 z} & -\mu S_3 e^{S_3 z} & \mu S_3 e^{-S_3 z}\end{pmatrix}\begin{pmatrix}1 & \frac{1}{\mu} & \frac{1}{S_1} & \frac{1}{\mu S_1}\\ 1 & \frac{1}{\mu} & \frac{-1}{S_1} & \frac{-1}{\mu S_1}\\ 1 & \frac{-1}{\mu} & \frac{1}{S_3} & \frac{-1}{\mu S_3}\\ 1 & \frac{-1}{\mu} & \frac{-1}{S_3} & \frac{1}{\mu S_3}\end{pmatrix} \tag{13}$$

$$A = \frac{1}{4}\begin{pmatrix}1 & 1 & 1 & 1\\ \mu & \mu & -\mu & -\mu\\ S_1 & -S_1 & S_3 & -S_3\\ \mu S_1 & -\mu S_1 & -\mu S_3 & \mu S_3\end{pmatrix}_l \begin{pmatrix} e^{S_1 z} & 0 & 0 & 0\\ 0 & e^{-S_1 z} & 0 & 0\\ 0 & 0 & e^{S_3 z} & 0\\ 0 & 0 & 0 & e^{-S_3 z}\end{pmatrix}\begin{pmatrix}1 & \frac{1}{\mu} & \frac{1}{S_1} & \frac{1}{\mu S_1}\\ 1 & \frac{1}{\mu} & \frac{-1}{S_1} & \frac{-1}{\mu S_1}\\ 1 & \frac{-1}{\mu} & \frac{1}{S_3} & \frac{-1}{\mu S_3}\\ 1 & \frac{-1}{\mu} & \frac{-1}{S_3} & \frac{1}{\mu S_3}\end{pmatrix} \tag{14}$$

which is valid for any translation $z$ over a region of constant scattering length density (and therefore $\mu$, $S_1$ and $S_3$), and is identical to the matrix in Eq. 128 of [1].

Because the wavefunction and first derivatives are continuous over any boundary, one can then use this transfer matrix to "advance" the wavefunction through an arbitrary number of layers, recalculating the matrix at each interface so that $S_1$, $S_3$ and $\mu$ are appropriate for the current layer.

$$\Psi_l = \left(\prod_{l=N}^{1} A_l\right)\Psi_0 \tag{15}$$

Using the additional boundary condition that the incident wave only comes from one direction, i.e.

$$C_{2,N} = C_{4,N} = D_{2,N} = D_{4,N} \equiv 0 \tag{16}$$

one can use this matrix product to calculate the reflectivity terms $r_{++}, r_{+-}, r_{-+}, r_{--}$.

## CONSTRUCTION OF TRANSFER MATRIX IN TERMS OF C COEFFICIENTS

It is possible to make an equivalent transfer matrix for the coefficients $C_j$, since they contain the same information as $\Psi$.

In order to do so we note that on either side of a boundary (between layer $l$ and layer $l+1$)

$$\Psi(z)_l = \Psi(z)_{l+1} \tag{17}$$

and plugging into Eq. 8

$$\begin{pmatrix} e^{S_1 z} & e^{-S_1 z} & e^{S_3 z} & e^{-S_3 z}\\ \mu_l e^{S_1 z} & \mu_l e^{-S_1 z} & -\mu_l e^{S_3 z} & -\mu_l e^{-S_3 z}\\ S_1 e^{S_1 z} & -S_1 e^{-S_1 z} & S_3 e^{S_3 z} & -S_3 e^{-S_3 z}\\ \mu_l S_1 e^{S_1 z} & -\mu_l S_1 e^{-S_1 z} & -\mu_l S_3 e^{S_3 z} & \mu_l S_3 e^{-S_3 z}\end{pmatrix}_l \begin{pmatrix}C_1\\ C_2\\ C_3\\ C_4\end{pmatrix}_l = \begin{pmatrix} e^{S_1 z} & e^{-S_1 z} & e^{S_3 z} & e^{-S_3 z}\\ \mu_l e^{S_1 z} & \mu_l e^{-S_1 z} & -\mu_l e^{S_3 z} & -\mu_l e^{-S_3 z}\\ S_1 e^{S_1 z} & -S_1 e^{-S_1 z} & S_3 e^{S_3 z} & -S_3 e^{-S_3 z}\\ \mu_l S_1 e^{S_1 z} & -\mu_l S_1 e^{-S_1 z} & -\mu_l S_3 e^{S_3 z} & \mu_l S_3 e^{-S_3 z}\end{pmatrix}_{l+1} \begin{pmatrix}C_1\\ C_2\\ C_3\\ C_4\end{pmatrix}_{l+1} \tag{18}$$

Applying the inverse matrix of the RHS gives a new $4\times4$ matrix $B$ that transfers $C_{j,l}$ to $C_{j,l+1}$.

$$\begin{pmatrix}C_1\\ C_2\\ C_3\\ C_4\end{pmatrix}_{l+1} = B_l\begin{pmatrix}C_1\\ C_2\\ C_3\\ C_4\end{pmatrix}_l \tag{19}$$

$$B_l = \frac{1}{4}\begin{pmatrix} e^{-S_1 z} & 0 & 0 & 0 \\ 0 & e^{S_1 z} & 0 & 0 \\ 0 & 0 & e^{-S_3 z} & 0 \\ 0 & 0 & 0 & e^{S_3 z} \end{pmatrix}_{l+1} \begin{pmatrix} 1 & \frac{1}{\mu} & \frac{1}{S_1} & \frac{1}{\mu S_1} \\ 1 & \frac{1}{\mu} & \frac{-1}{S_1} & \frac{-1}{\mu S_1} \\ 1 & \frac{-1}{\mu} & \frac{1}{S_3} & \frac{-1}{\mu S_3} \\ 1 & \frac{-1}{\mu} & \frac{-1}{S_3} & \frac{1}{\mu S_3} \end{pmatrix}_{l+1} \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mu & \mu & -\mu & -\mu \\ S_1 & -S_1 & S_3 & -S_3 \\ \mu S_1 & -\mu S_1 & -\mu S_3 & \mu S_3 \end{pmatrix}_l \begin{pmatrix} e^{S_1 z} & 0 & 0 & 0 \\ 0 & e^{-S_1 z} & 0 & 0 \\ 0 & 0 & e^{S_3 z} & 0 \\ 0 & 0 & 0 & e^{-S_3 z} \end{pmatrix}_l \tag{20}$$

TABLE I. Elements of the $B$-matrix, which transfers $C_{j,l} \to C_{j,l+1}$

$$\begin{aligned}
B_{11} &= \tfrac{1}{4}e^{(S_{1,l}-S_{1,l+1})z}\left(1+\tfrac{\mu_l}{\mu_{l+1}}+\tfrac{S_{1,l}}{S_{1,l+1}}+\tfrac{\mu_l S_{1,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{12} &= \tfrac{1}{4}e^{(-S_{1,l}-S_{1,l+1})z}\left(1+\tfrac{\mu_l}{\mu_{l+1}}-\tfrac{S_{1,l}}{S_{1,l+1}}-\tfrac{\mu_l S_{1,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{13} &= \tfrac{1}{4}e^{(S_{3,l}-S_{1,l+1})z}\left(1-\tfrac{\mu_l}{\mu_{l+1}}+\tfrac{S_{3,l}}{S_{1,l+1}}-\tfrac{\mu_l S_{3,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{14} &= \tfrac{1}{4}e^{(-S_{3,l}-S_{1,l+1})z}\left(1-\tfrac{\mu_l}{\mu_{l+1}}-\tfrac{S_{3,l}}{S_{1,l+1}}+\tfrac{\mu_l S_{3,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{21} &= \tfrac{1}{4}e^{(S_{1,l}+S_{1,l+1})z}\left(1+\tfrac{\mu_l}{\mu_{l+1}}-\tfrac{S_{1,l}}{S_{1,l+1}}-\tfrac{\mu_l S_{1,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{22} &= \tfrac{1}{4}e^{(-S_{1,l}+S_{1,l+1})z}\left(1+\tfrac{\mu_l}{\mu_{l+1}}+\tfrac{S_{1,l}}{S_{1,l+1}}+\tfrac{\mu_l S_{1,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{23} &= \tfrac{1}{4}e^{(S_{3,l}+S_{1,l+1})z}\left(1-\tfrac{\mu_l}{\mu_{l+1}}-\tfrac{S_{3,l}}{S_{1,l+1}}+\tfrac{\mu_l S_{3,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{24} &= \tfrac{1}{4}e^{(-S_{3,l}+S_{1,l+1})z}\left(1-\tfrac{\mu_l}{\mu_{l+1}}+\tfrac{S_{3,l}}{S_{1,l+1}}-\tfrac{\mu_l S_{3,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{31} &= \tfrac{1}{4}e^{(S_{1,l}-S_{3,l+1})z}\left(1-\tfrac{\mu_l}{\mu_{l+1}}+\tfrac{S_{1,l}}{S_{3,l+1}}-\tfrac{\mu_l S_{1,l}}{\mu_{l+1}S_{3,l+1}}\right)\\
B_{32} &= \tfrac{1}{4}e^{(-S_{1,l}-S_{3,l+1})z}\left(1-\tfrac{\mu_l}{\mu_{l+1}}-\tfrac{S_{1,l}}{S_{3,l+1}}+\tfrac{\mu_l S_{1,l}}{\mu_{l+1}S_{3,l+1}}\right)\\
B_{33} &= \tfrac{1}{4}e^{(S_{3,l}-S_{3,l+1})z}\left(1+\tfrac{\mu_l}{\mu_{l+1}}+\tfrac{S_{3,l}}{S_{3,l+1}}+\tfrac{\mu_l S_{3,l}}{\mu_{l+1}S_{3,l+1}}\right)\\
B_{34} &= \tfrac{1}{4}e^{(-S_{3,l}-S_{3,l+1})z}\left(1+\tfrac{\mu_l}{\mu_{l+1}}-\tfrac{S_{3,l}}{S_{3,l+1}}-\tfrac{\mu_l S_{3,l}}{\mu_{l+1}S_{3,l+1}}\right)\\
B_{41} &= \tfrac{1}{4}e^{(S_{1,l}+S_{3,l+1})z}\left(1-\tfrac{\mu_l}{\mu_{l+1}}-\tfrac{S_{1,l}}{S_{1,l+1}}+\tfrac{\mu_l S_{1,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{42} &= \tfrac{1}{4}e^{(-S_{1,l}+S_{3,l+1})z}\left(1-\tfrac{\mu_l}{\mu_{l+1}}+\tfrac{S_{1,l}}{S_{1,l+1}}-\tfrac{\mu_l S_{1,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{43} &= \tfrac{1}{4}e^{(S_{3,l}+S_{3,l+1})z}\left(1+\tfrac{\mu_l}{\mu_{l+1}}-\tfrac{S_{3,l}}{S_{1,l+1}}-\tfrac{\mu_l S_{3,l}}{\mu_{l+1}S_{1,l+1}}\right)\\
B_{44} &= \tfrac{1}{4}e^{(-S_{3,l}+S_{3,l+1})z}\left(1+\tfrac{\mu_l}{\mu_{l+1}}+\tfrac{S_{3,l}}{S_{1,l+1}}+\tfrac{\mu_l S_{3,l}}{\mu_{l+1}S_{1,l+1}}\right)
\end{aligned}$$

The components of $B$ are listed in Table I. While this approach doesn't reduce the complexity of the calculation of $r$ and $t$, it does offer advantages in the case of DWBA problems; no extra work is done converting between $\Psi$ and $C_j$ at every layer, and the DWBA terms depend on $\int_{z_l}^{z_{l+1}} \Psi(z)$ which is much easier to calculate as $\int_{z_l}^{z_{l+1}} \sum_j C_{j,l} e^{S_{j,l} z}$ than $\left(\int_{z_l}^{z_{l+1}} A_l(z)\right) \Psi(z = z_l)$.

The calculation of $r$ can by setting the incident polarization to $\pm 1$ and using the equations

$$\begin{aligned} C_{2,N} &= B_{21}C_{1,0} + B_{22}C_{2,0} + B_{23}C_{3,0} + B_{24}C_{4,0} \equiv 0 \\ C_{4,N} &= B_{41}C_{1,0} + B_{42}C_{2,0} + B_{43}C_{3,0} + B_{44}C_{4,0} \equiv 0 \end{aligned} \tag{21}$$

noting that

$$\begin{aligned} C_{1,0} &\equiv I_+ \\ C_{2,0} &\equiv r_+ \\ C_{3,0} &\equiv I_- \\ C_{4,0} &\equiv r_- \end{aligned} \tag{22}$$

giving expressions for $r$

$$\begin{aligned} r_{++} &= \tfrac{B_{24}B_{41} - B_{21}B_{44}}{B_{44}B_{22} - B_{24}B_{42}} \\ r_{+-} &= \tfrac{B_{21}B_{42} - B_{41}B_{22}}{B_{44}B_{22} - B_{42}B_{24}} \\ r_{-+} &= \tfrac{B_{24}B_{43} - B_{23}B_{44}}{B_{44}B_{22} - B_{24}B_{42}} \\ r_{--} &= \tfrac{B_{23}B_{42} - B_{43}B_{22}}{B_{44}B_{22} - B_{42}B_{24}} \end{aligned} \tag{23}$$

then the transmission can be calculated, since we now know all the $C_{j,0}$, and

$$\begin{aligned} t_+ &\equiv C_{1,N} \\ t_- &\equiv C_{3,N} \end{aligned} \tag{24}$$

## ROTATION OF REFERENCE FRAME

The equations in the previous section were derived in a single reference frame, which for the sample is defined by convention to have $\hat{z}_{\text{SAM}} \parallel \vec{Q}$. Given that the $\hat{z}$ direction is also by convention the quantization axis for spin, we have to apply a transformation if the lab quantization axis ($\hat{z}_{\text{LAB}} \parallel \vec{H}_{\text{guide}}$) is not collinear with $\hat{z}_{\text{SAM}}$.

In order to mate the laboratory reference frame to the sample one, we have to do a rotation. As per Eq. 3.2.46 in [2], a spinor is rotated about an axis according to

$$\chi \to \exp\left(\frac{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi}{2}\right)\chi \tag{25}$$

The rotation matrix around the $\hat{x}$-axis is (as in [1])

$$U_R = \begin{pmatrix} \cos(\epsilon/2) & i\sin(\epsilon/2) & 0 & 0 \\ i\sin(\epsilon/2) & \cos(\epsilon/2) & 0 & 0 \\ 0 & 0 & \cos(\epsilon/2) & i\sin(\epsilon/2) \\ 0 & 0 & i\sin(\epsilon/2) & \cos(\epsilon/2) \end{pmatrix} \tag{26}$$

The wavefunction in the incident medium has no coupling between $\psi_+$ and $\psi_-$ when $\rho_{+-}, \rho_{-+} = 0$. In practice, we take the wavefunction in the incident medium and rotate it from the lab frame to the sample frame, and then just inside the first layer of the sample we can calculate the $C_j$.

$$\begin{aligned} U_R^{-1}\Psi_{\mathrm{LAB}} &= \Psi_{\mathrm{SAM}} \\ \chi^{-1}U_R^{-1}\Psi_{\mathrm{LAB}} &= \chi^{-1}\Psi_{\mathrm{SAM}} = \begin{pmatrix} C_j \end{pmatrix} \end{aligned} \tag{27}$$

If one wishes to calculate the wavefunction in the laboratory frame throughout the sample, within each layer the solutions for $C_j$ can transferred to the lab frame by noting that

$$\begin{pmatrix} \psi_+(z) \\ \psi_-(z) \end{pmatrix}_{\mathrm{LAB}} = U_R \begin{pmatrix} \psi_+(z) \\ \psi_-(z) \end{pmatrix}_{\mathrm{SAM}}$$

$$= \begin{pmatrix} \cos(\epsilon/2)[\sum_j C_j e^{S_j z}] + i\sin(\epsilon/2)[\sum_j \mu_j C_j e^{S_j z}] \\ i\sin(\epsilon/2)[\sum_j C_j e^{S_j z}] + \cos(\epsilon/2)[\sum_j \mu_j C_j e^{S_j z}] \end{pmatrix} \tag{28}$$

and collecting terms that all have the same $e^{S_j z}$ dependence, we get

$$\begin{aligned} C^{\uparrow}_{j,\mathrm{LAB}} &= (\cos(\epsilon/2) + i\mu_j \sin(\epsilon/2))\, C_{j,\mathrm{SAM}} \\ C^{\downarrow}_{j,\mathrm{LAB}} &= (\mu_j \cos(\epsilon/2) + i \sin(\epsilon/2))\, C_{j,\mathrm{SAM}} \end{aligned} \tag{29}$$

Within the DWBA layer-by-layer calculations, of course, the reference frame doesn't matter as long as $\langle\psi_f|$ and $|\psi_i\rangle$ are in the same reference frame, and it will be easiest to use the $\begin{pmatrix} C_j \end{pmatrix}$ in the sample frame.

* brian.maranville@nist.gov

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[2] J. Sakurai, *Modern Quantum Mechanics (Rev. Ed.)* (Addison Wesley Longman, INC., USA, 1994).